

Quantum Molecular Dynamics

Simulating Warm, Dense Matter

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Regions of warm, dense matter abound—from the interiors of giant gaseous planets, such as Saturn, and the atmospheres of white dwarf stars to laboratory plasmas in high-energy density generators and inertial confinement fusion capsules. Warm, dense matter, a sizzling “soup” of atoms, molecules, ions, and free electrons, is difficult to describe by standard techniques because it harbors multiple species and processes simultaneously—from ionization and recombination to molecular dissociation and association. Recently, quantum molecular dynamics (QMD), which can predict static, dynamical, and optical properties from a single, first principles framework, has been used to accurately predict properties of hydrogen, oxygen-nitrogen mixtures, and plutonium in the warm, dense state.

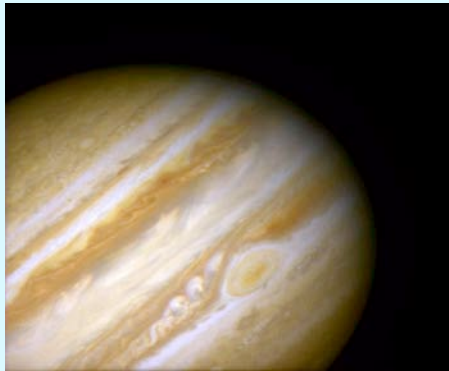


At the core of Saturn,
there is warm, dense matter,
ranging between 5000 and
6000 kelvins in temperature.

Abstract: QMD

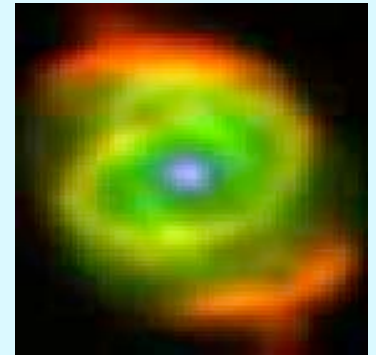
The need to better model the regimes of warm, dense matter [10^2 - 10^6 K; $0.01 - 100$ g/cm³] in which quantal behavior, especially for the electrons, becomes important, has received new impetus from many areas including weapons science and planetary modeling as well as shock-compression and high-energy-density physics. To meet these needs, we have applied quantum molecular dynamics (QMD) methods, which join the latest flavor of Density Functional Theory for the electrons to the classical equations of motion for the nuclei, to a variety of systems and conditions. Examples include static (EOS), dynamical, and optical properties of 1) mixtures [H/He, N/O, Ti/H, SiO₂, Li/F]; 2) shocked materials [Ga, Sn, Fe]; and 3) temporally-evolving samples [e.g. Au] after short-pulse laser irradiation. In addition to providing a basic understanding of the interaction mechanisms, the exploration of mixtures also tests popular models for mixing the properties of the pure species to obtain those of the composite. For the shocked materials, we also examine possible signatures in the optical properties of various phase changes. The third example highlights a push into new physical realms by extending the method to non-equilibrium conditions for coupling of the electron and ion components.

We have developed larger-scale classical and quasi-classical molecular dynamics techniques to treat ultracold multi-component plasmas and Rydberg gases in external fields. Such systems, produced by traps using similar technology as for Bose-Einstein Condensates, can serve as effective laboratories to explore many basic plasma processes. In addition, with an added magnetic field, we have studied the conditions within the ATOM and Athena antihydrogen experiments at CERN with the goal of devising mechanisms to de-excite the high Rydberg states currently produced to low-lying levels that can be spectroscopically probed to determine possible deviations from CPT symmetry and to discriminate among different gravitational theories

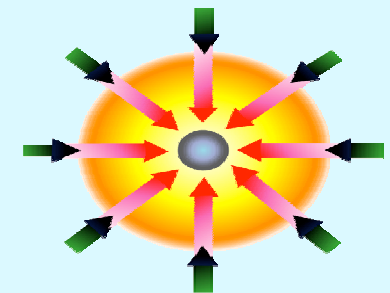
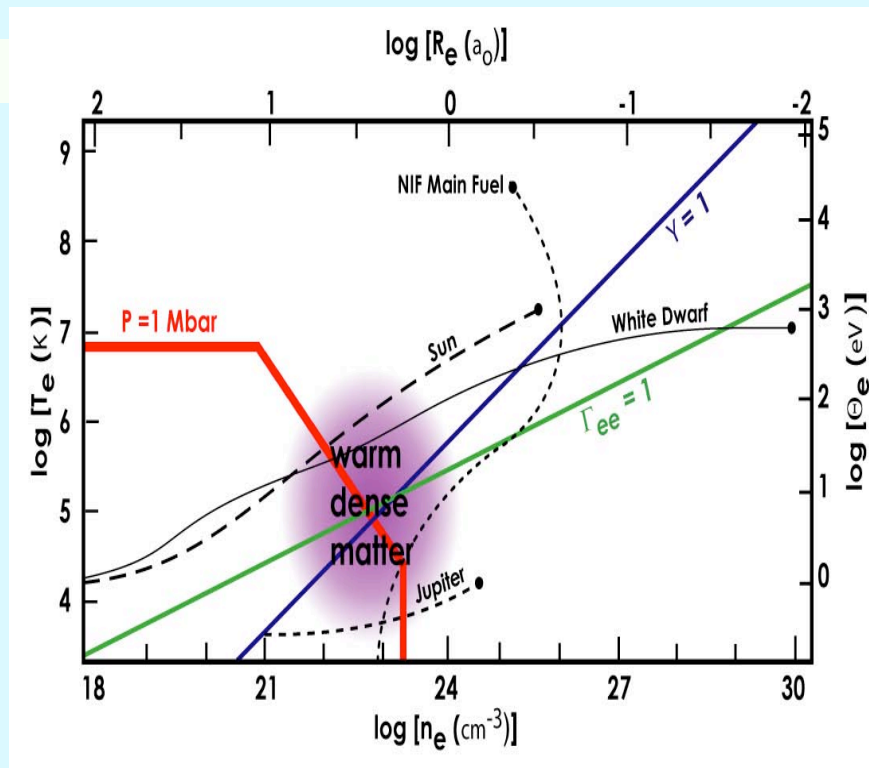


Giant & Extrasolar Planets

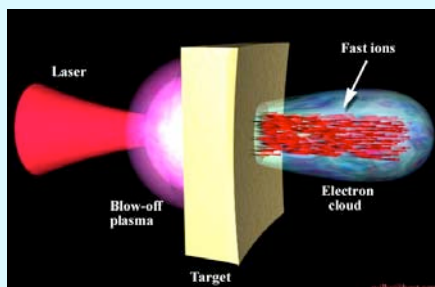
Applications



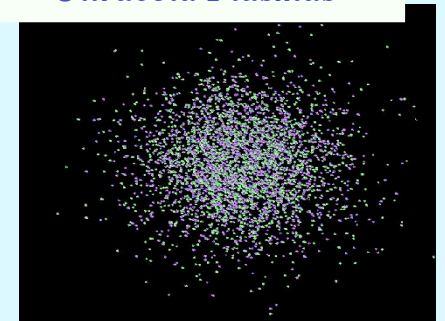
Stellar Atmospheres



High-energy Density Media



Ultracold Plasmas



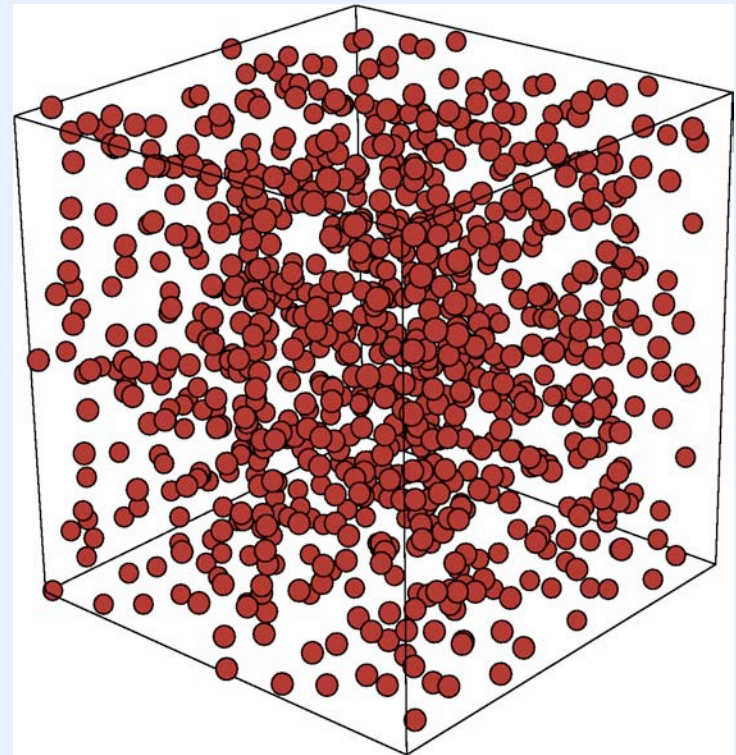
Quantum Simulations

snapshot

- **3D Periodic Cell: N atoms**
- **Born-Oppenheimer**
- **Electrons: Quantum mechanical treatment:**

$$H\Psi = E \Psi$$

*dissociation, association, ionization,
recombination*



Nuclear Motion: $F = ma$

Quantum Molecular Dynamics

Consistent set of Properties: $\{R_i, P_i\}$, $\Psi(r_i; R_i)$

- **Static:** EOS, pressure, internal energy
- **Dynamical:** Diffusion, thermal conductivity, viscosity
- **Optical:** Electrical conductivity, opacity, reflectivity

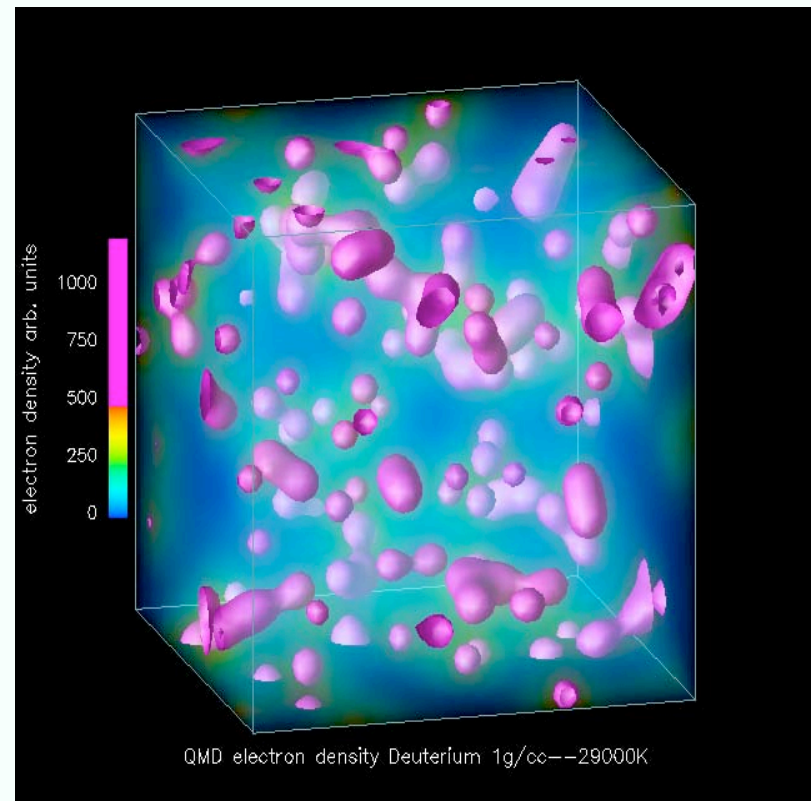
Quantum Simulations

- **Tight-Binding Molecular Dynamics (TB):**
Semi-empirical
- **Density Functional MD:** “ab initio” (DFT)
Local density (LDA),
Generalized Gradient Approximation (GGA),
Hybrid
- **Path Integral Monte Carlo (PIMC):**
Quantum statistical mechanic

Theory & Computation

Finite-Temperature Density Functional Theory

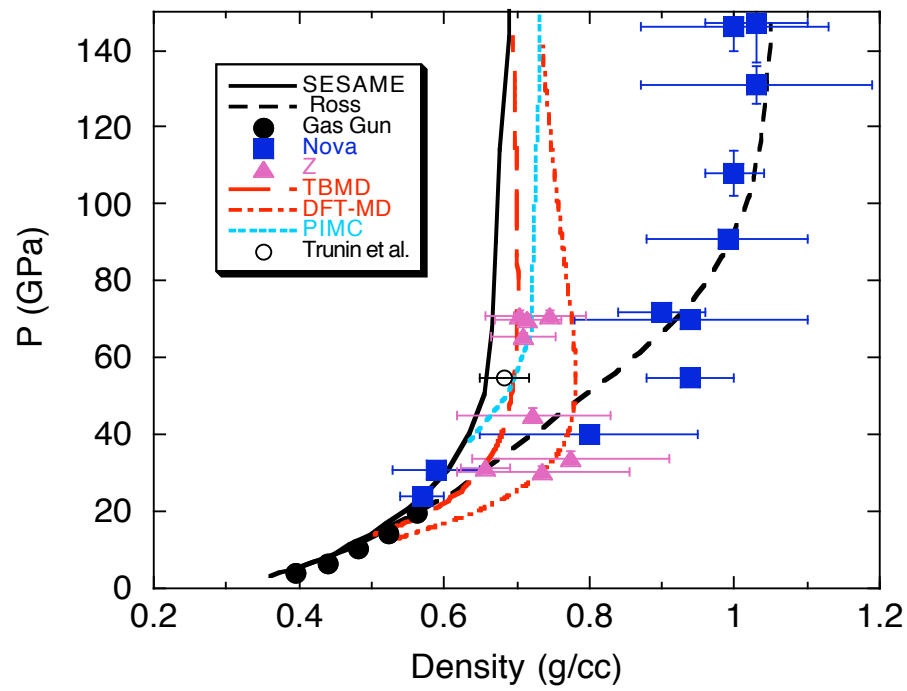
- Generalized Gradient Approximation (GGA)
- Plane-Wave Basis
- Pseudopotential (TM/Ultrasoft)
- Projector Augmented Wave (PAW)
- K-point integration
- LTE ($T_e = T_{ion}$)
- $N \sim 100 - 1000$



Natural Limits

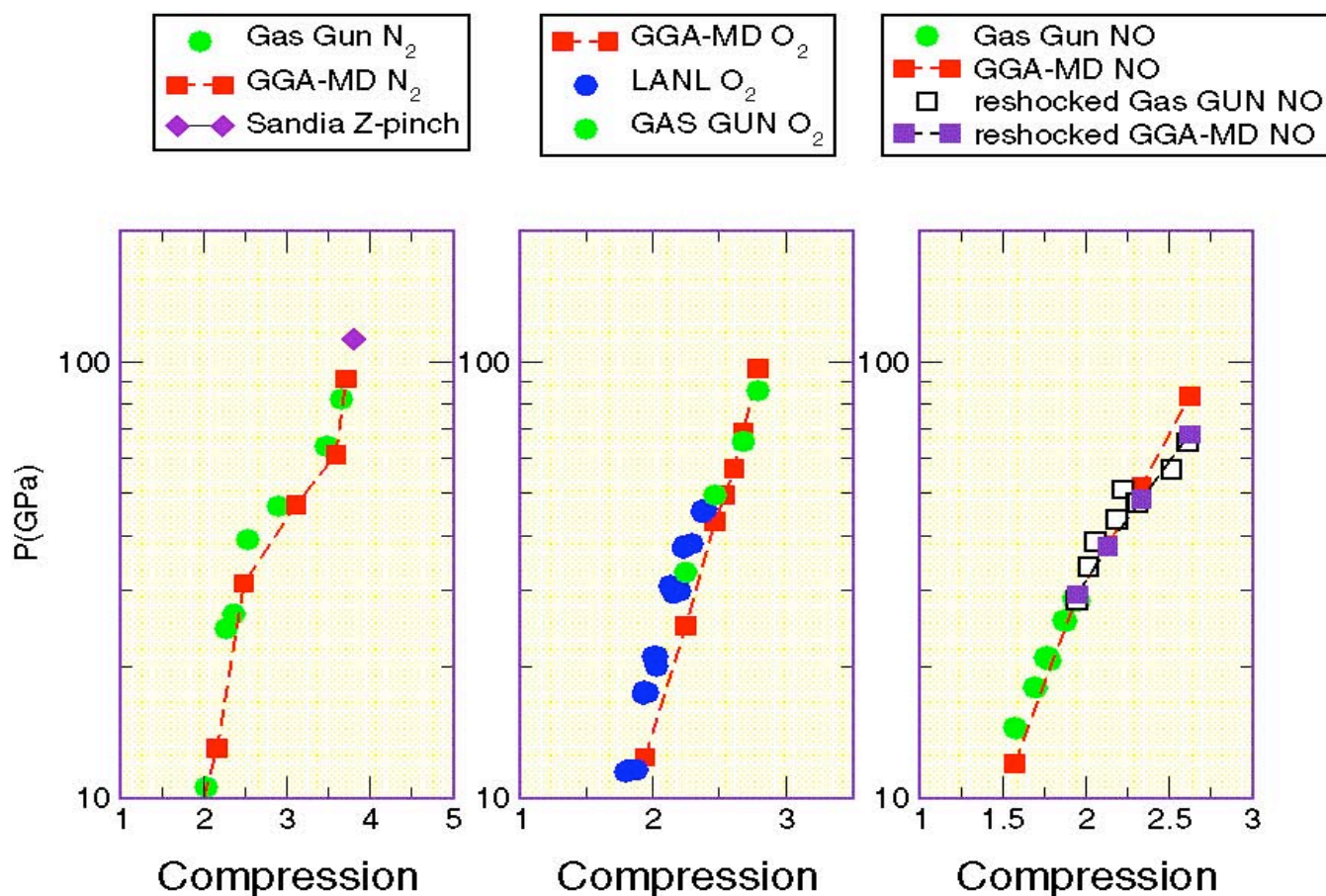
Static Properties

Deuterium Hugoniot

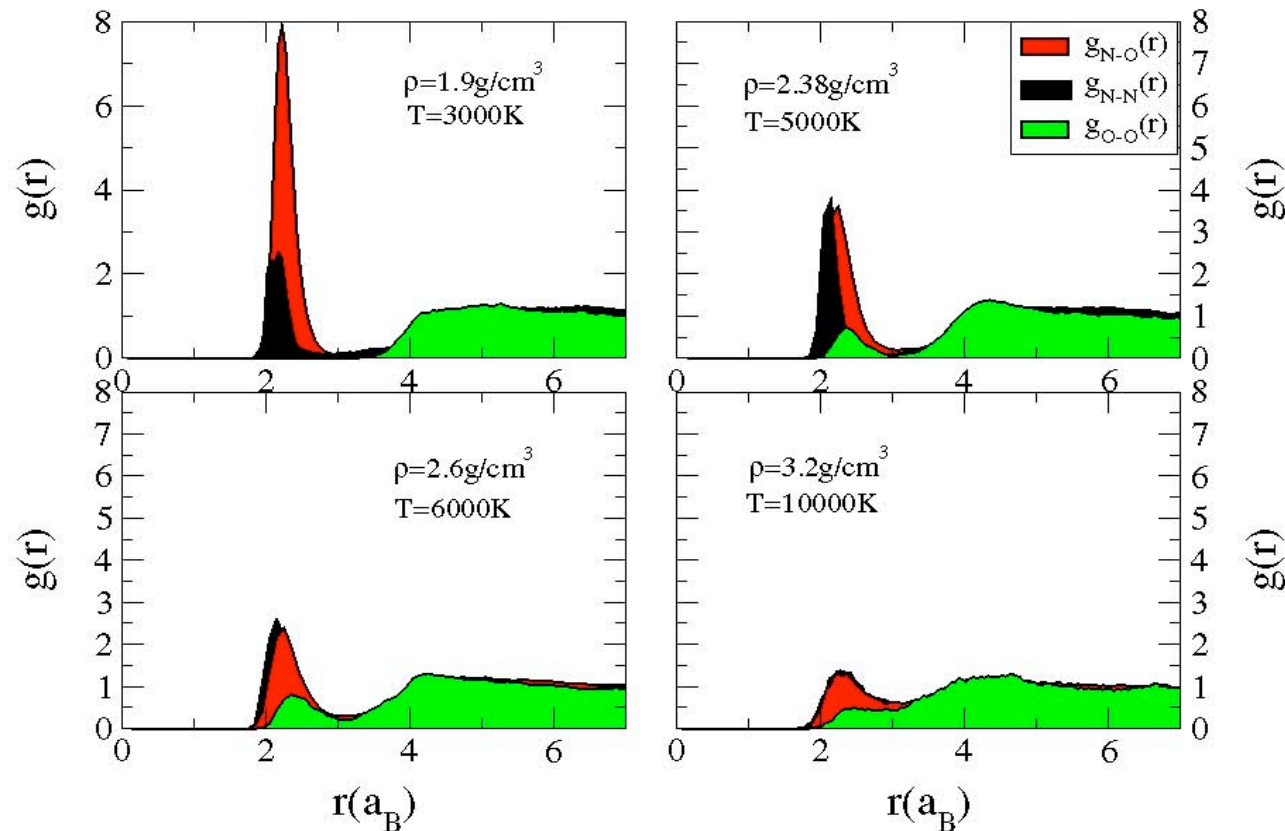


Hugoniot: N_2 , O_2 , NO

Validation: MD-DFT(GGA) and Experiment

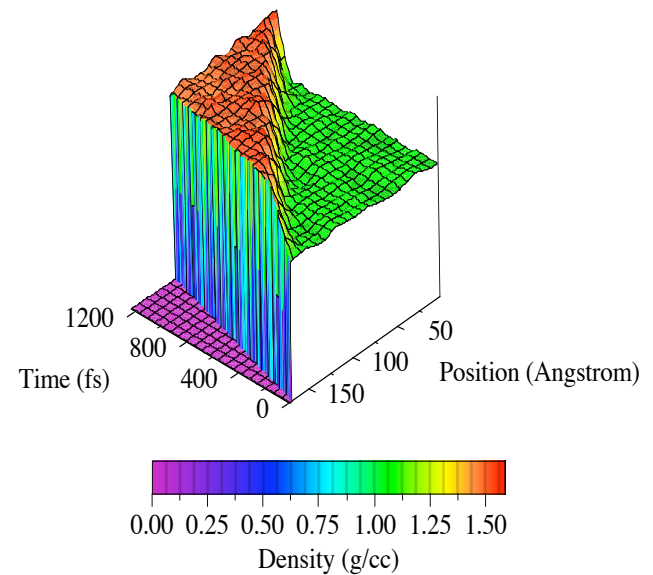
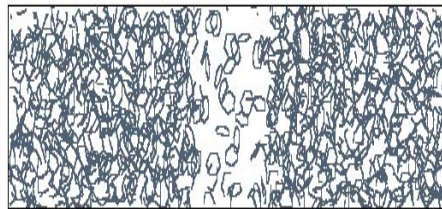
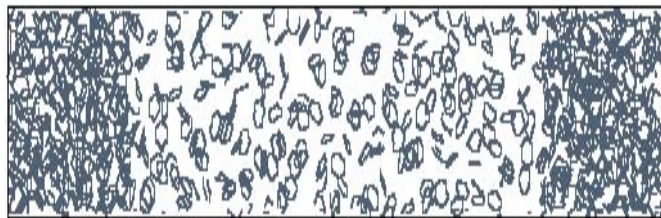


Composition along Principal Hugoniot

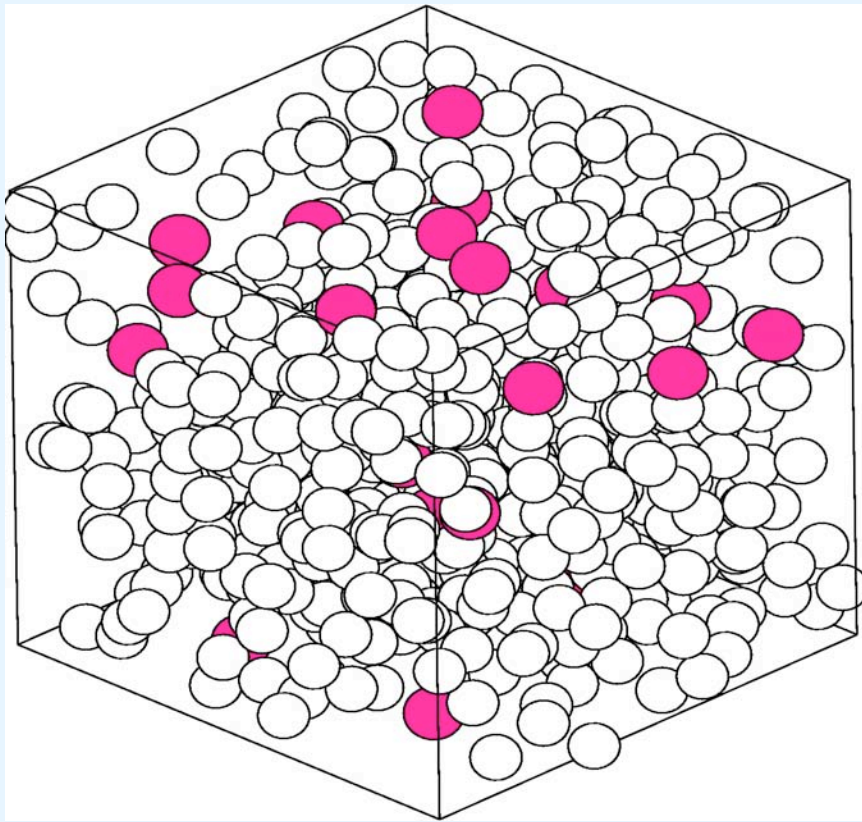


Mazevet, Blottiau, Kress, & Collins, Phys. Rev. B **69**, 224207 (2004)

Dynamical Properties:



Hydrogen/Titanium Mixtures



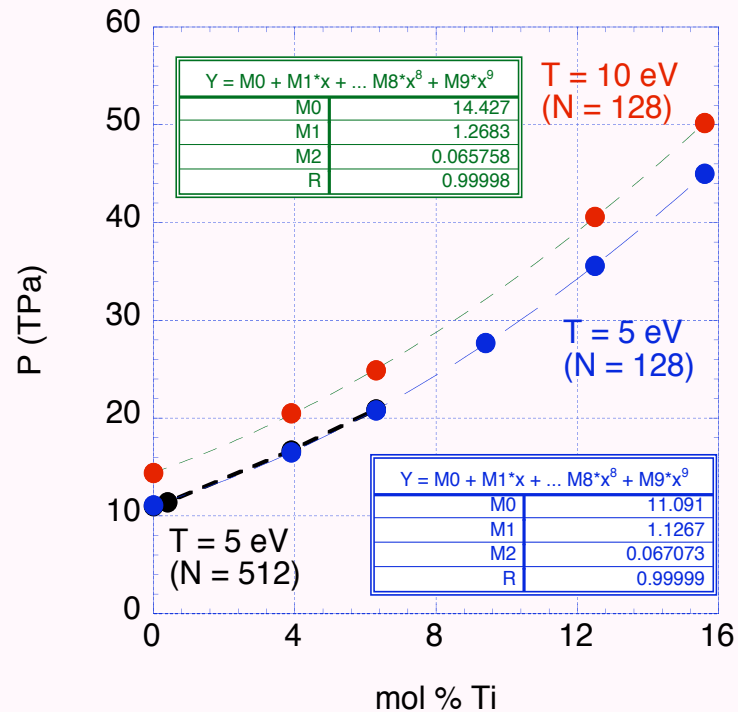
Density = 5g/cc

$\text{H}_{492}\text{Ti}_{20}$ (3.9% Ti)

Hydrogen/Titanium Mixtures

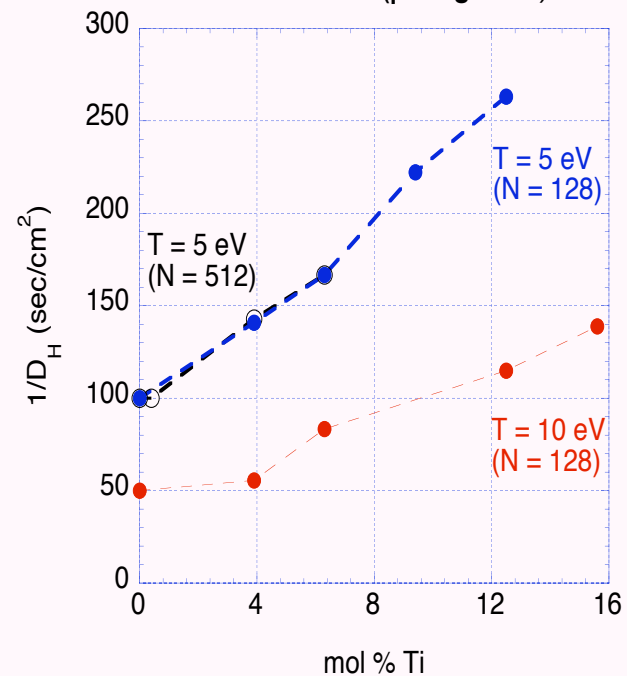
Equation of State

H/Ti "Plasma" ($\rho = 5 \text{ g/cm}^3$)



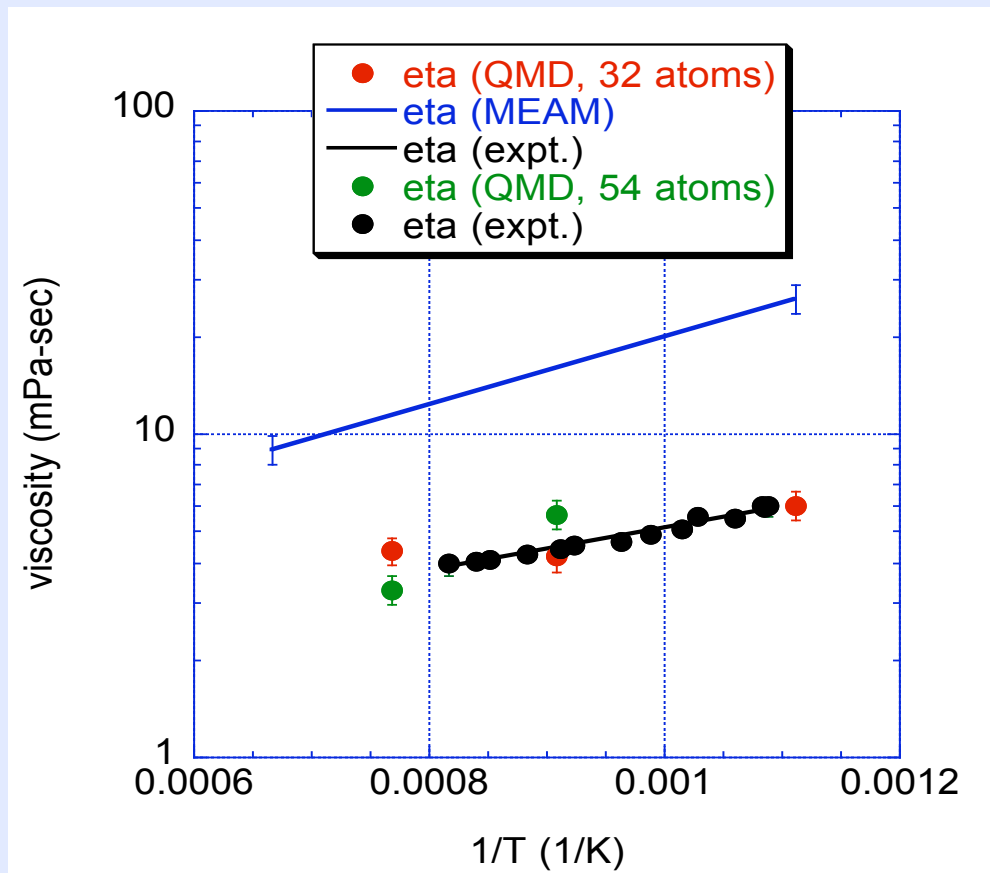
Inverse Hydrogen Self-Diffusion Coefficient

H/Ti "Plasma" ($\rho = 5 \text{ g/cm}^3$)

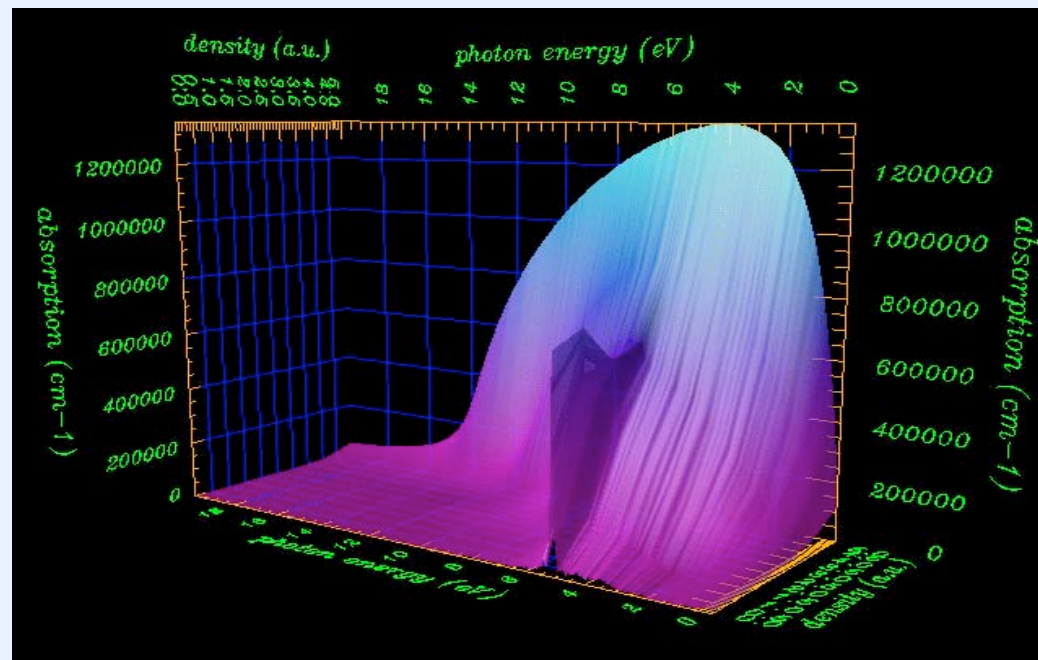


QMD: Pu Viscosity

$$\eta(T) = \frac{k_b T}{D(T) d} \times \text{constant}$$

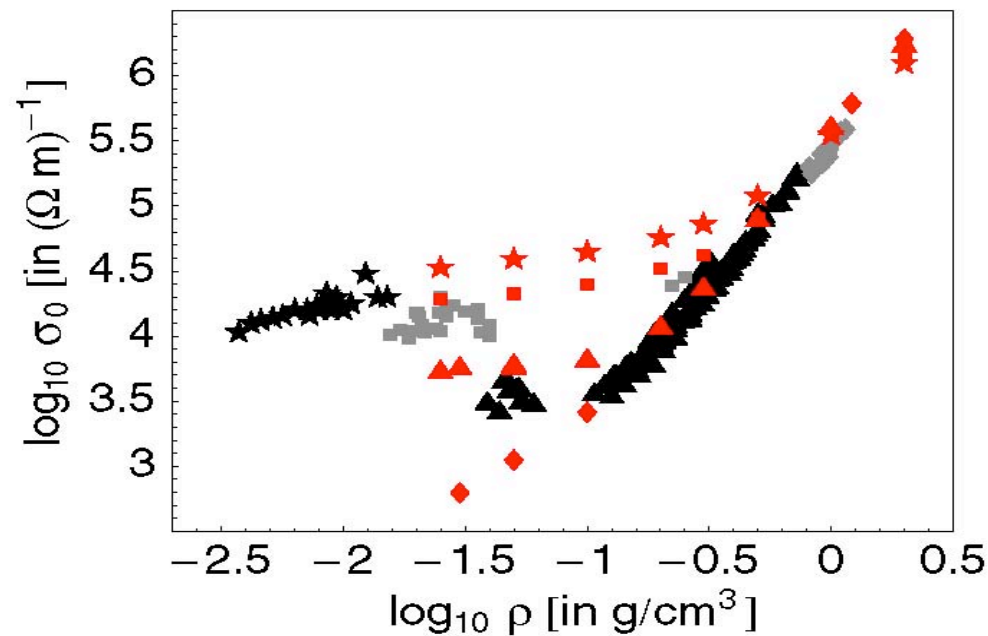


Optical Properties:



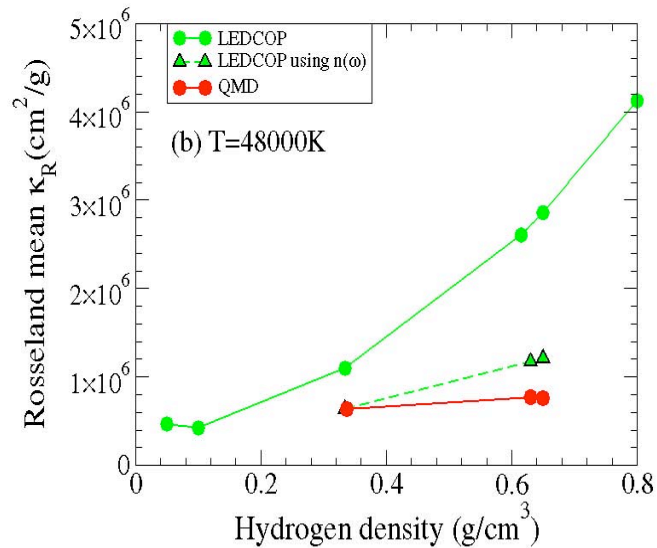
Aluminum: Electrical Conductivity

QMD vs Experiment



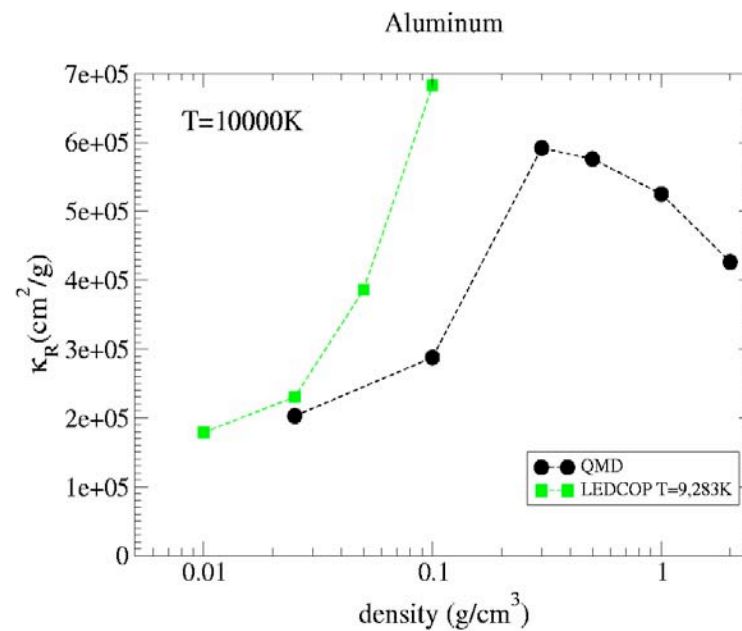
Mazevet , Desjarlais, Collins, Kress, & Magee, Phys. Rev. E **71**, 016409 (2005)

Rosseland Mean Opacity: QMD & LEDCOP



Hydrogen (H)

Aluminum (Al)



Mazevet, Collins, Magee, Kress, & Keady *Astron. Astrophys. Lett.* **405**, L5 (2003)

Future Directions:

- **Non-equilibrium**
[ion-electron coupling]
- **Optical properties**
[TDDFT/RPA]
- **External Fields**
- **Experimental Validation**
- **Predictive capabilities:**
new regimes

